## **CONDENSED MATTER, MATERIALS SCIENCE, and CHEMISTRY**

## Large and Rapid Deformation of Dense Particulate Composite

Xia Ma, Qisu Zou, Duan Z. Zhang, and W. Brian VanderHeyden, T-3; and Nely Padial-Collins, CCS-2

anufacturing and application of dense particulate composite material under large deformation and shock loading have profound interest at this Laboratory. For instance, it is found that the manufacturing processes significantly affect mechanical properties of the material. Interaction of energetic grains in an explosive material during the material failure may result in safety hazards. During the failure and manufacturing process, the composite behaves like a dense granular flow since the binder is either very weak or the grains have debonded from the binder. To obtain the capability of predicting the complicated phenomena and assessing safety risk, we developed a statistical theory for dense granular material. Numerical simulations are performed to study the material under various deformations loading conditions. We investigated the effect of lubrication effects of polymeric binder during the manufacturing process. Our results indicate that significant improvement of the product quality can be achieved by increasing temperature to reduce the viscosity of the polymeric binder. As shown in Fig. 1, slight reduction of friction between grains can significantly reduce stress relaxation time of the composite. Figure 2 shows the stressstrain relation under repeated loading and unloading cycles in the simulation of the manufacturing process for different friction coefficients between particles.

Figure 3 shows the crack propagation in the particulate material under a horizontal uniaxial tension. A small vertical initial crack was at the

center of the figure. The traditional continuum theory predicts that the crack propagates along the center line. This figure clearly demonstrates that the path of crack propagation deviates significantly from the predicted path. Thus, to study the fracture properties of the particulate material, a statistical theory for dense granular material is essential.

To investigate effects of grain deformations and binder flow under a high-pressure environment, one needs to study how multiphase interactions involving binder, crystal, and product gas form chemical reactions. This is a typical case of the class of very difficult problems known as fluid-structure interactions. To meet these challenges, we implemented the particle-in-cell (PIC) method into the code CartaBlanca to take advantage of both Lagrangian and Eulerian methods, while avoiding their disadvantages such as numerical diffusion in the Eulerian method and mesh tangling in the Lagrangian method. CartaBlanca is a general multiphase numerical simulation package we developed using the object-oriented language Java and an advanced solver technique. The features of the Java language enable us to easily implement many practical engineering material models, and to perform parallel calculations easily. This code has proven successful in many important applications and has won a 2005 R&D 100 award. Figure 4 shows a simulation of shock traveling through a particulate composite consisting of binder and grains. At rest (velocity is zero) binders are in blue and grains are yellow. Red is superimposed on the colors of the grains and the binder to represent the velocities of the material. Red represents the velocity corresponding to 2.5 Mach in the grains and 10 Mach in the binder. These detailed numerical results will enable us to study energy dissipation mechanisms in the material deemed to be critically important in the study of such materials.

## **CONDENSED MATTER, MATERIALS SCIENCE, and CHEMISTRY**

For more information contact Xia Ma at xia@lanl.gov.

## **Funding Acknowledgements**

The Joint DoD/DOE Munitions Technology Development Program.

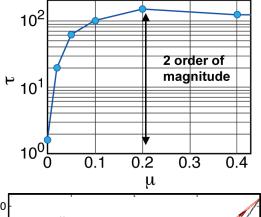


Fig. 1. Stress relaxation as a function of friction between particles.

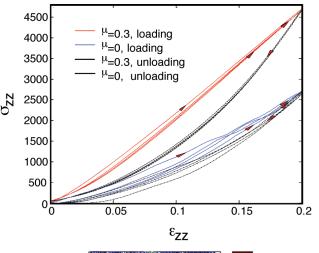


Fig. 2. Stress-strain relation under cyclical compression for different frictions between particles.

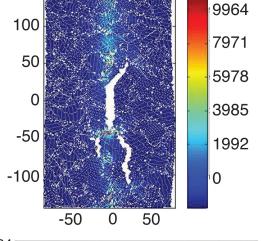


Fig. 3. Crack propagation in a particulate material.

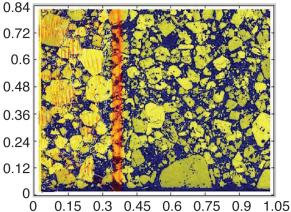


Fig. 4. A shock wave traveling through a particulate composite.

